

Polarons in the harmonic lattice.

I. Standing polaron.

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Abstract

We obtain analytical expressions for the large- and small-radius polarons on the one-dimensional lattice in the TBA approximation. The equations of motion for this model are treated classically for the oscillator subsystem, while a quantum description is used for the electron. The electron-phonon interaction is considered in the linear Su–Schrieffer–Heeger approximation. Good agreement between analytical formulae and accurate numerical simulation is obtained. The dynamics of polaron formation from different initial conditions is considered. Some features of the wave function evolution, governed by the finite lattice length, are elucidated.

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I. INTRODUCTION

Charge and energy transfer is of utmost importance in both organic and inorganic nature. Studies of charge transport (CT) in organic systems were restricted till recently by research of amorphous state. CT in individual quasi-one-dimensional systems has attracted much attention. These oligo- and macromolecules have some advantages compared to traditional bulk systems because of less size, flexibility and power requirements. Biopolymers like natural and synthetic DNA, and proteins [1–4] are of particular interest. These systems can find an applications in solar cells, flexible TV displays, logical circuits etc. [5–9]. Molecular electronics can also be used in the nanotechnology [10–16]. Photosynthesis, ATP hydrolysis, metabolism are examples where CT is vitally important [17–19].

Polarons are ubiquitous in materials where the electron-phonon coupling cannot be ignored. Polarons are thought to be responsible for the CT in biological systems [20–22] including DNA. Different DNA models were considered to describe the polaron properties [23–27]. Dozens of papers present results on the effects of water and counterions surrounding DNA, on polaron properties in the presence of disorder, polaron hopping and drift in an applied electric field [24, 28–39].

Polarons in the harmonic lattice are thoroughly investigated in the resent paper. The electron-phonon interaction is described in terms of the linear Su–Schrieffer–Heeger approximation in the tight-binding modelling. Analytical expressions for small and large polarons are derived. Results coincide with numerical simulation with high accuracy. The dynamics of polaron formation from different initial conditions is considered. An influence of the lattice finite size on the wave function evolution is also analyzed.

II. THE SMALL-RADIUS POLARON IN THE HARMONIC LATTICE

A. Numerical simulation

The one-dimensional harmonic lattice with one extra charge carrier is investigated. We consider an electron for the definiteness though the arguing is valid for the holes. The lattice consists of N particles. The "particle" represents one base of DNA in the coarse-grained model of DNA. The TBA approximation is used to describe the electron evolution on the lattice.

The hamiltonian of this system is the sum of the classical hamiltonian and the energy of electron-phonon interaction:

$$H = \frac{m}{2} \sum_{i=1}^N \dot{x}_i^2 + \frac{k}{2} \sum_{i=1}^{N-1} (x_{i+1} - x_i)^2 + \left\langle \vec{\Psi} | \hat{H}^e | \vec{\Psi} \right\rangle, \quad (1)$$

where x_i is the deviation of i -th particle from the equilibrium, $\vec{\Psi} = \psi_1, \psi_2, \dots$ is the electron wave function. m and k are the particle mass and the lattice rigidity, respectively. In the TBA approximation the electron hamiltonian is the tridiagonal matrix:

$$\hat{H}^e = \begin{pmatrix} e_1 & t_1 & 0 & 0 & \dots & 0 & 0 \\ t_1 & e_2 & t_2 & 0 & \dots & 0 & 0 \\ 0 & t_2 & e_3 & t_3 & \dots & 0 & 0 \\ 0 & 0 & t_3 & e_4 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & e_{N-1} & t_{N-1} \\ 0 & 0 & 0 & 0 & \dots & t_{N-1} & e_N \end{pmatrix} \quad (2)$$

where t_i is the hopping integral and e_i is the electron on-site energy. In the homogeneous lattice all diagonal elements are equal and can be set to zero, $e_i = 0$. The hopping integral is written in the Su-Schrieffer-Heeger form [27, 40]:

$$t_i = -[v_0 - \alpha(x_{i+1} - x_i)]. \quad (3)$$

This model mimics the synthetic DNA or peptide consisting of the regular sequence of identical bases or peptide groups (see e.g. [41]).

It is convenient to consider hamiltonian (1) in the dimensionless quantities. Let us choose the following units: v_0 is the energy unit, $\sqrt{m k^{-1}}$ is the time unit and $\sqrt{v_0 k^{-1}}$ is the length unit. Then the dimensionless hamiltonian is

$$H = \frac{1}{2} \sum_{i=1}^N \dot{x}_i^2 + \frac{1}{2} \sum_{i=1}^{N-1} q_i^2 - \sum_{i=1}^{N-1} (1 - \alpha q_i) (\psi_i^* \psi_{i+1} + \text{c.c.}), \quad (4)$$

where the same notation is preserved for the dimensionless variables; $q_i \equiv (x_{i+1} - x_i)$ is the relative displacement of the neighboring particles. The dimensionless parameter $\alpha/\sqrt{k v_0} \rightarrow \alpha$ is the free parameter. Below we study the one-dimensional polaron solutions of the hamiltonian (4).

We find the solution for the standing stationary polaron when all velocities in (4) $\dot{x}_i = 0$. The minimum of energy (4) with respect to all lattice variables $\{q_i\}$ and the electronic wave function $\{\psi_i\}$ determines the polaron.

If Eq. (4) is minimized with respect to $\{\psi_i\}$ then $\vec{\Psi}$ is the eigenfunction of the electronic hamiltonian \hat{H}^e with energy ε . It means that two procedures, – energy minimization and solving the stationary Schrödinger equation, are equivalent.

The electron wave function oscillates as $\psi_i e^{i\varepsilon t/\hbar}$, where $\{\psi_i\}$ are real amplitudes of electron wave function. Note, the time oscillations are eliminated in (4) because of complex conjugation. Then the expression for the energy (4) is

$$H = \frac{1}{2} \sum_{i=1}^{N-1} q_i^2 - 2 \sum_{i=1}^{N-1} (1 - \alpha q_i) \psi_i \psi_{i+1}. \quad (5)$$

The minimization (5) (i.e. $\partial H / \partial q_i = 0$) gives

$$q_i = -2\alpha \psi_i \psi_{i+1}. \quad (6)$$

Substitution of (6) into (5) results in:

$$H = -2 \sum_{i=1}^{N-1} \psi_i \psi_{i+1} - 2\alpha^2 \sum_{i=1}^{N-1} (\psi_i \psi_{i+1})^2. \quad (7)$$

An analogous approach was used in [21].

Expression (7) was minimized numerically preserving the norm $\sum_i \psi_i^2 = 1$. If the lattice length N is much larger than the polaron radius then the polaron solution does not depend on N . The numerical steepest descent method was used to find the polaron profile on the lattice with $N = 101$. The result is shown in Fig. 1a.

This polaron is centered on the particle. Such polarons will be called the *site* polarons hereafter. The polaron center can be located on the center of the bond between two nearest particles. Such polarons are called *intersite* polarons. The energy is somewhat higher in the latter case (see Fig. 1b).

Small energy difference of the site and intersite polarons can be treated as the barrier separating two spatially different polaron states with equal energies. The typical value for the energy unit in DNA is $v_0 = 0.3$ eV. Then the energy difference between site and intersite polarons is as small as $\lesssim 0.0001$ eV. This small energy difference points to the possibility of ballistically travelling polarons. This finding can also be the starting point for contraction of translationally-invariant states.

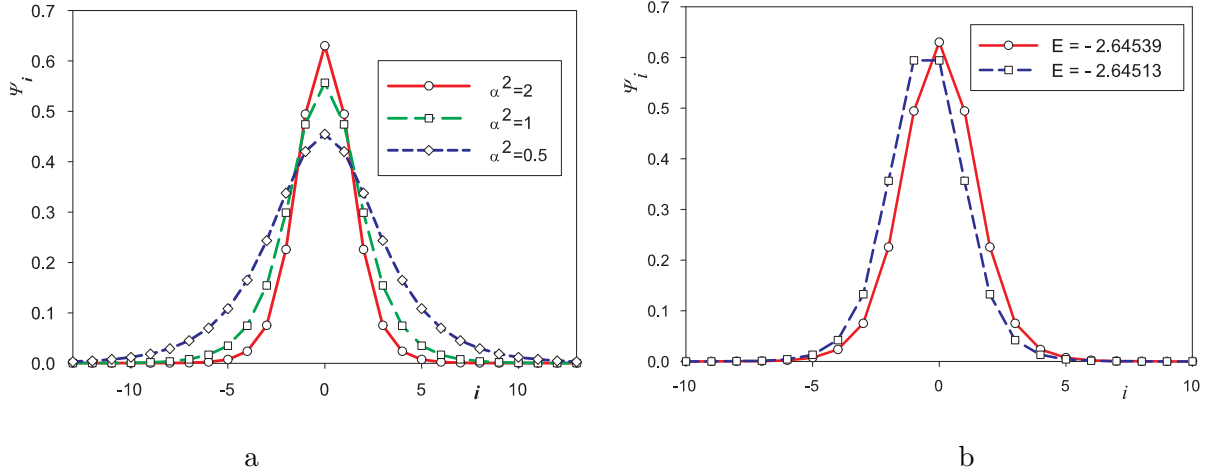


FIG. 1: Results of the numerical calculations of the polaron. a) Wave functions for three values of parameter α (shown in insert). b) Site (solid line) and intersite (dashed line) polarons for $\alpha^2 = 2$. Energies of these polarons are shown in insert to the figure. Polarons are centered at the site $i = 0$ ($-50 \leq i \leq 50$) in both figures.

The total lattice contraction $\Delta L = \sum_i q_i$, and using (6) one finds

$$\Delta L = -2\alpha \sum_{i=1}^{N-1} \psi_i \psi_{i+1}. \quad (8)$$

For large-width polaron $\psi_i \approx \psi_{i+1}$ and taking into account the norm of the wave function (i.e. $= 1$) $\Delta L \approx 2\alpha$.

B. Analytical expressions for the small-radius polaron

For definiteness we consider the site polarons hereafter. The wave function of polaron is symmetrical relative to its center. Consequently only one-half of a polaron (say, right half) can be analyzed. This problem is considered on the semi-infinite lattice and the new site numeration is used: $i = 0, 1, 2, \dots, \infty$. The amplitudes of the wave function are denoted as ψ_0 for the central polaron site and ψ_i , $i = 1, 2, \dots$ for other sites. Then the expression for energy (7) is transformed to

$$H = -4 \sum_{i=0}^{\infty} \psi_i \psi_{i+1} - 4\alpha^2 \sum_{i=0}^{\infty} (\psi_i \psi_{i+1})^2 \quad (9)$$

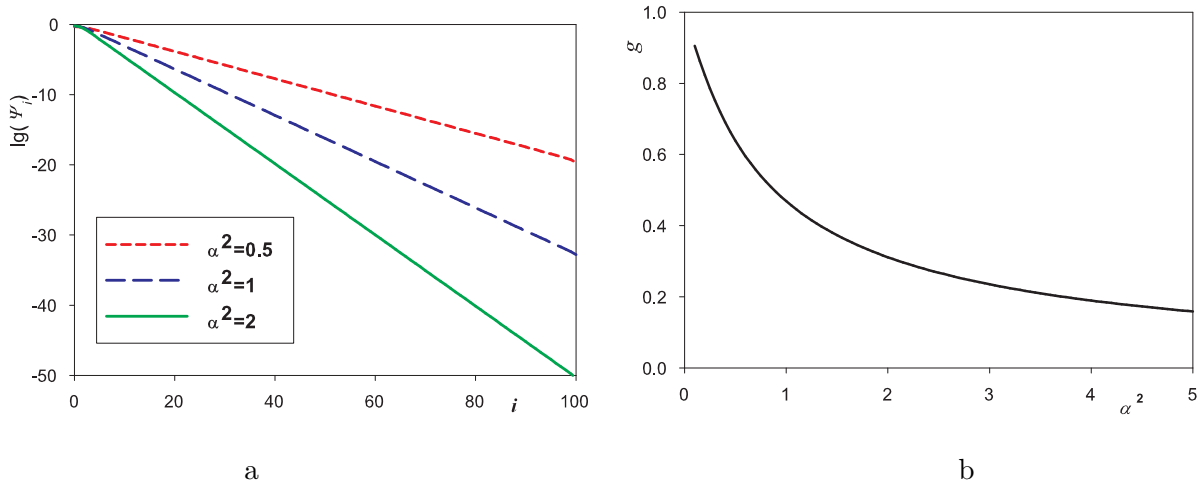


FIG. 2: a) Exponential decay of the wave function for different values of α . $N = 201$. b) The dependence of parameter g vs. α .

with the rescaled norm of the wave function

$$\psi_0^2 + 2 \sum_{i=1}^{\infty} \psi_i^2 = 1. \quad (10)$$

Numerical minimization of energy (9) with respect to all ψ_i shows that the wave function decreases exponentially with the growth of i when $i \gg 1$ (see Fig. 2a), i.e. $\psi_i \propto \exp(-i/R)$ and R is the polaron radius.

It is convenient to introduce parameter g related to the radius R by

$$R = \frac{1}{\ln g}. \quad (11)$$

This relation follows from the exponential decay of the wave function amplitude: $\psi_i \propto g^i$ at $i \gg 1$. In other words, g is the common ratio of the geometrical progression: $g = \psi_{i+1}/\psi_i$. Fig. 2b shows the dependence of g vs. parameter α of electron-phonon interaction. One can see that the value of g approaches unity for $\alpha \rightarrow 0$ and the polaron radius increases when parameter α decreases.

The analytical solution can be constructed employing the asymptotic behavior of the wave function at large i . Our goal is to express the wave function and parameter α through g .

It is convenient to introduce the Lagrange multiplier μ to find the energy minimum of (9). It allows to take into account the condition for preserving the norm of wave function

(10). Then the minimization of the functional

$$\tilde{H} = H + \mu \left(\psi_0^2 + 2 \sum_{i=1}^{\infty} \psi_i^2 - 1 \right) \quad (12)$$

with respect to $\psi_0, \psi_1, \psi_2, \dots$ gives the following system of equations

$$\begin{cases} \psi_1 + 2\alpha^2 \psi_0 \psi_1^2 = \frac{\mu}{2\psi_0} \\ \psi_{i+1} + \psi_{i-1} + 2\alpha^2 \psi_i (\psi_{i+1}^2 + \psi_{i-1}^2) = \mu \psi_i; \quad i \geq 1 \end{cases} \quad (13)$$

The Lagrange multiplier μ is expressed through g as

$$\mu \approx g + \frac{1}{g}. \quad (14)$$

This relation follows from the second equation (13) which becomes linear for $i \gg 1$: $\psi_{i+1} + \psi_{i-1} = \mu \psi_i$. The solution of this equation is $\psi_i \propto g^i$. It can be also verified that $\mu = -\varepsilon$ where ε is the electronic contribution to the polaron energy.

The construction of the approximate analytical polaron solution will be performed in the following manner. We suppose that the exponential decay for the solution is a good approximation starting from some site number i_0 . It means that the cubic terms in (13) can be neglected.

At the zeroth approximation the exponential decay starts from ψ_0 ($i_0 = 0$) and $\psi_i = \psi_0 g^i$. This is very rough approximation and we consider two next approximations.

1. Polaron solution in the first approximation

The exponential decay of the wave function starts from $i_0 = 1$ in the first approximation. And amplitudes are: $\psi_0, \psi_1, \psi_2 = \psi_1 g, \psi_3 = \psi_1 g^2, \dots$. Then only two equations for ψ_0 and ψ_1 remain in (13):

$$\begin{cases} \psi_1 + 2\alpha^2 \psi_0 \psi_1^2 = \frac{\mu}{2} \psi_0 \\ \psi_1 g + \psi_0 + 2\alpha^2 \psi_1 (\psi_0^2 + g^2 \psi_1^2) = \mu \psi_1. \end{cases} \quad (15)$$

An expression for the norm of the wave function is

$$\psi_0^2 + 2 \frac{\psi_1^2}{1 - g^2} = 1 \quad (16)$$

and the second term in (16) is calculated as a sum of terms of infinite geometrical progression.

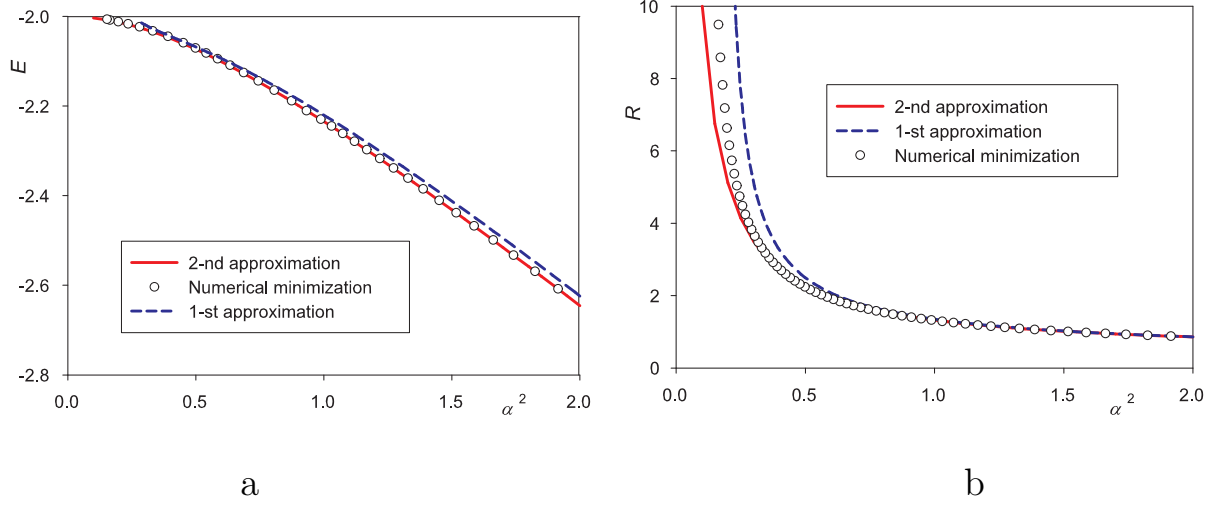


FIG. 3: a) Polaron energy *vs.* parameter α of electron-phonon interaction in the first and second approximations. b) The polaron radius R *vs.* parameter α . Results of numerical minimization are shown in empty circles. $N = 101$.

As a result we get three algebraic equations (15) and (16) for three variables ψ_0, ψ_1 and α . The exact solution is too cumbersome and is not given. There exists a limiting case when term $(g\psi_1)^2$ in (15) is neglected. This approximation corresponds to the accuracy of the first approximation. The answer in this case is very simple:

$$\psi_0 = \sqrt{\frac{1-g^2}{2}}; \quad \psi_1 = \frac{\sqrt{1-g^4}}{2}. \quad (17)$$

An expression for α is obtained by substitution (17) and (14) into the first of equations (15). The polaron energy, expressed through ψ_0, ψ_1 and α , is

$$E = -4 \left[\psi_0 \psi_1 + \frac{g\psi_1^2}{1-g^2} + \alpha^2 \psi_1^2 \left(\psi_0^2 + \frac{g^2 \psi_1^2}{1-g^4} \right) \right]. \quad (18)$$

The comparison of the results obtained in the first approximation with the "exact" (numerical) results is shown in Fig. 3. There is some discrepancy and the next approximation is required.

2. Polaron solution in the second approximation

The exponential decay of amplitudes in the second approximation starts from $i_0 = 2$. Amplitudes of wave function are: $\psi_0, \psi_1, \psi_2, \psi_3 = \psi_2 g, \psi_4 = \psi_2 g^2, \dots$ and form the geometrical

progression starting from the third term. Three equations

$$\begin{cases} \psi_1 + 2\alpha^2\psi_0\psi_1^2 = \frac{\mu}{2}\psi_0 \\ \psi_2 + \psi_0 + 2\alpha^2\psi_1(\psi_0^2 + \psi_2^2) = \mu\psi_1 \\ g\psi_2 + \psi_1 + 2\alpha^2\psi_2(\psi_1^2 + g^2\psi_2^2) = \mu\psi_2 \end{cases} \quad (19)$$

from system (13) is enough to solve the problem in the second approximation. The normalizing condition for the wave function is

$$\psi_0^2 + 2\psi_1^2 + 2\frac{\psi_2^2}{1-g^2} = 1. \quad (20)$$

Algebraic equations (19) and (20) are solved numerically. The solution for the wave function is a series. First three terms (ψ_0, ψ_1, ψ_2) are obtained from the solution of these equations. Next terms $(\psi_i, i \geq 3)$ are members of the geometrical progression with the common ratio g .

The comparison of "exact" (numerical minimization) and results obtained in the second approximation is shown in Figs. 3a and 3b. One can see that the coincidence is very good.

III. THE LARGE-RADIUS POLARON

The parameter α of electron-phonon interaction determines the radius of polaron: polaron has large radius if α is small. In this case the common ratio g in the geometrical progression is close to unity. We shall find the solution for the large-radius polaron in the continuous approximation on the infinite lattice $(-\infty < i < \infty)$.

The starting point for the evaluating the solution is the same as in the case of small-radius polaron. Let us write this equation once more for convenience:

$$\psi_{i+1} + \psi_{i-1} + 2\alpha^2\psi_i(\psi_{i+1}^2 + \psi_{i-1}^2) = \mu\psi_i. \quad (21)$$

g is slightly less than unity for the large-radius polaron, and the Lagrange multiplier μ ($\mu = g + 1/g$) is somewhat larger than 2. Let's introduce small parameter $\delta^2 \equiv \mu - 2$ and make some transformations in Eq. (21). Firstly, subtract $2\psi_i$ from both sides of Eq. 21:

$$\frac{1}{\delta^2}(\psi_{i+1} + \psi_{i-1} - 2\psi_i) + 2\frac{\alpha^2}{\delta^2}\psi_i(\psi_{i+1}^2 + \psi_{i-1}^2) = \psi_i. \quad (22)$$

Next, $(\psi_{i+1}^2 + \psi_{i-1}^2)$ can be substituted by $2\psi_i^2$ because the difference between the amplitudes of the wave function on neighboring sites is very small for the large-radius polaron. As a result we get

$$\frac{1}{\delta^2}(\psi_{i+1} + \psi_{i-1} - 2\psi_i) + 4\frac{\alpha^2}{\delta^2}\psi_i^3 = \psi_i. \quad (23)$$

And, finally, we introduce new variables: $y_i = \frac{\alpha\sqrt{2}}{\delta}\psi_i$. As a result the following equation is obtained:

$$\frac{1}{\delta^2}(y_{i+1} + y_{i-1} - 2y_i) + 2y_i^3 = y_i. \quad (24)$$

First term in the left hand side of (24) is the difference form of the second derivative. Applying the continuous approximation the following equation is obtained:

$$y'' = y + 2y^3. \quad (25)$$

Its solution is

$$y = \frac{1}{\cosh(x)} \quad \text{or} \quad \psi(x) = \frac{\delta}{\alpha\sqrt{2}} \frac{1}{\cosh(x)}. \quad (26)$$

The normalization of the wave function gives $\delta = \alpha^2$, then the final expression for the large-radius polaron in discrete form is

$$\psi_i = \frac{\alpha}{\sqrt{2}} \frac{1}{\cosh(\alpha^2 i)}. \quad (27)$$

Very similar solution is obtained for a somewhat analogous problem in [23].

The comparison of “exact” results (numerical minimization) and the analytical expression (27) is shown in Fig. 4 for two values of parameter α . The agreement is very good and it is the better the larger is polaron radius. In one dimension case there is a transition from the small to the large polaron and $\alpha \approx 0.6$ separates these two solutions.

IV. THE DYNAMICS OF POLARON FORMATION

Two cases of large and small polarons were considered above. These solutions correspond to the energy minimum in the stationary state. And now we consider the evolution of the dynamical and electronic degrees of freedom giving the polaron as the final state.

The following numerical experiment was performed. The wave function with some profile was chosen as the initial electronic condition. Initial conditions for the dynamical variables: lattice at rest, i.e. $x_i = 0$, $\dot{x}_i = 0$.

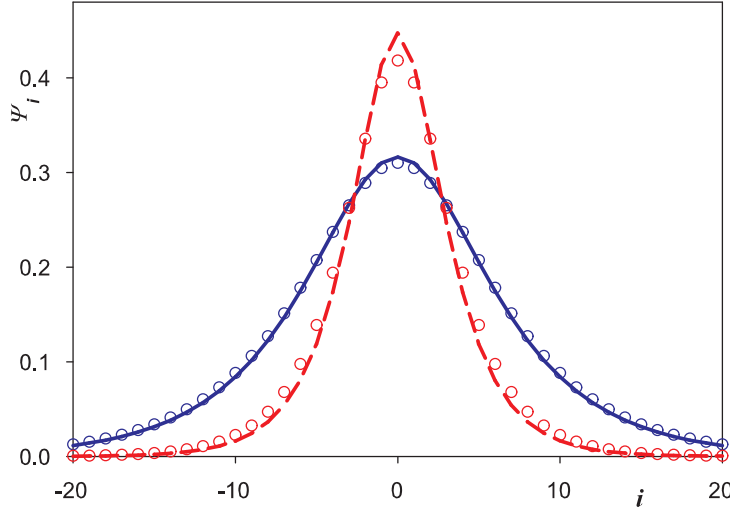


FIG. 4: The dependence of the amplitudes of wave function vs. the site number i according to (27). Dashed line – for $\alpha = 0.4$, solid line – for $\alpha = 0.2$. Circles – accurate results of numerical minimization.

The system evolution is determined by the following system

$$\begin{cases} \ddot{x}_i = (x_{i-1} + x_{i+1} - 2x_i) + \alpha[(\psi_i \psi_{i+1}^* + \psi_i^* \psi_{i+1}) - (\psi_{i-1} \psi_i^* + \psi_{i-1}^* \psi_i)] \\ \dot{\psi}_i = \frac{i}{\tilde{h}} [(1 - \alpha q_i) \psi_{i-1} + (1 + \alpha q_i) \psi_{i+1}] \end{cases} \quad (28)$$

where $q_i \equiv (x_{i+1} - x_i)$ and \tilde{h} is the dimensionless Planck's constant: $\frac{\hbar}{v_0} \sqrt{\frac{m}{k}} \rightarrow \tilde{h}$. If DNA parameters are chosen [20] then $1/\tilde{h} \approx 80$.

If the wave function is initially located on one site ($\psi_i(t=0) \propto \delta_{i,i_0}$), or has the constant value on the lattice ($\psi_i(t=0) \propto N^{-1/2}$), then the wave function spreads over lattice very rapidly and polarons are not formed. The reason is that the characteristic electronic time is very small ($\sim \tilde{h} \approx 10^{-2}$) compared to the dynamical time scale (~ 1). And the dynamical degrees of freedom have no enough time to follow the wave function.

If the initial wave function is chosen as a eigenfunction of unperturbed lattice, then the lattice “captures” the oscillating electron and the joint electron-lattice evolution results in polaron formation. The trial complex wave function is chosen in the form $\psi_i^0(t=0) = \left(\sqrt{\frac{2}{N+1}} \sin \left[\frac{\pi i}{N+1} \right], 0 \right)$. It corresponds to the ground-state wave function of the unperturbed lattice. The evolution of the wave function is shown in Fig. 5. The

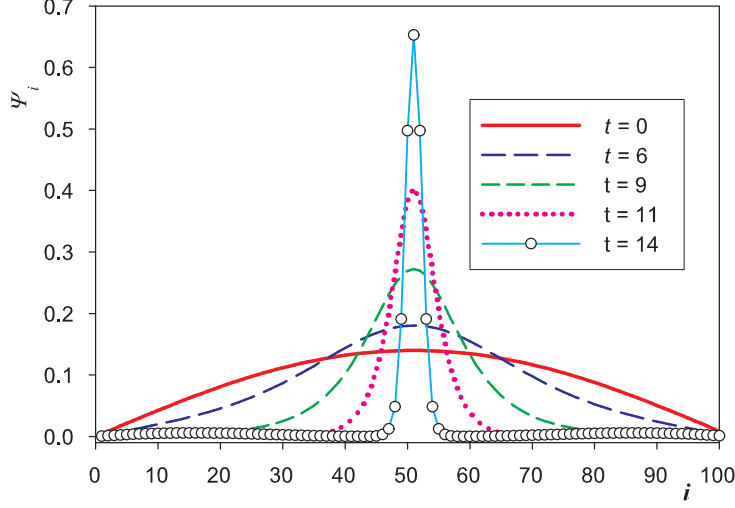


FIG. 5: Snapshots of the wave function evolution at different time instances shown in insert. Initial wave function $\psi_i(t=0) \propto (\sin[\pi i/(N+1)], 0)$. $\alpha^2 = 2, N = 101$. At $t = 14$ the polaron is completely formed.

polaron is formed during few oscillation periods of the lattice.

Eqs (28) correspond to the microcanonical ensemble where total energy is preserved. The energy gain due to the polaron formation is compensated by the vibrational excitation of a lattice. Because of the dynamical interaction with the lattice, polaron fluctuates, slightly changes its form and position, but stays very stable. If frictional forces at the lattices ends $-\gamma\dot{x}_1$ and $-\gamma\dot{x}_N$ are introduced then all vibrations decay and only polaron survives on the lattice.

If the initial wave function is the eigenfunction of the first excited state $\psi_i^1(t=0) = \left(\sqrt{\frac{2}{N+1}} \sin \left[\frac{2\pi i}{N+1} \right], 0 \right)$ then *two* polarons are formed but with norm of wave function = 0.5 for each of them.

The problem of charge transfer from a donor to the DNA double strand is very complex quantum-dynamical problem. An accurate solution of of time dependent Schrödinger equation for coupled state of excited donor and a lattice is necessary. We did not touch this problem here and limited ourself by the model representation of the initial wave functions.

V. WAVE FUNCTION EVOLUTION ON THE FINITE-SIZED LATTICE

Polarons on the infinite lattice were considered in the previous sections. But if the particular applications of the suggested approach are of interest (e.g. charge transfer in DNA) then the lattice should have the finite length, i.e. $N \lesssim 100$. And there appears few peculiarities which differ the polaron dynamics on the infinite lattice from the lattice of final length. Few examples are considered below.

First of all, the intriguing property of the evolution equations (28) should be mentioned. At some initial conditions the interaction of an electron with the lattice is the “one-way”: There exists an influence of the lattice on the electron through electron-phonon interaction, but the back “polaronic” action of an electron on the lattice is absent. In other words, additional forces acting on particles from the electron subsystem are zeroes. In the simplest case it is realized if the wave function is initially localized on one (arbitrary) site. Let the initial wave function for definiteness is real and totally located on the first site: $\psi_1(t=0) = 1$. From the second set of equations (28) it follows that at the certain time step the wave function on odd sites is real, and on even sites is imaginary. At the next time step the situation inverts: the wave function on odd sites is imaginary, and on even sites is real. Then the products $\psi_i \psi_{i+1}^*$ is always zero (see (28)). Hence, the lattice always stays to be harmonic. This conclusion is also valid if the initial wave function is organized in such a manner that it is real on all even sites and imaginary on all odd sites (or vice versa).

Second interesting case is the wave function evolution on the inhomogeneous lattice. Let one (arbitrary) lattice site i_0 has the TBA parameters which differs from others. These parameters are $\tilde{e}_{i_0} \neq 0$ for the electron on-site interaction, and $\tilde{\alpha} \neq \alpha$ for the electron-phonon interaction (3). Initial wave function can be chosen arbitrary. If the wave function for the homogeneous lattice ($\tilde{e} = 0, \tilde{\alpha} = \alpha$) never forms the localized state – polaron, but for the lattice with defect the case is opposite: the polaron is formed after some induction period. The result is shown in Fig. 6a. Though the norm of the polaron wave function is less than unity, polaron stays a stable quasiparticle for a very long time.

The polaron formation can be observed as follows: The maximal value of the wave function amplitude is monitored and this maximum is averaged over some time interval. The formation of the stable maximum with $\max|\psi| = 0.5 - 0.6$ is the direct evidence of the polaron formation (see Fig. 6b). Polaron is formed practically instantaneously at $\tilde{\alpha} = 1$,

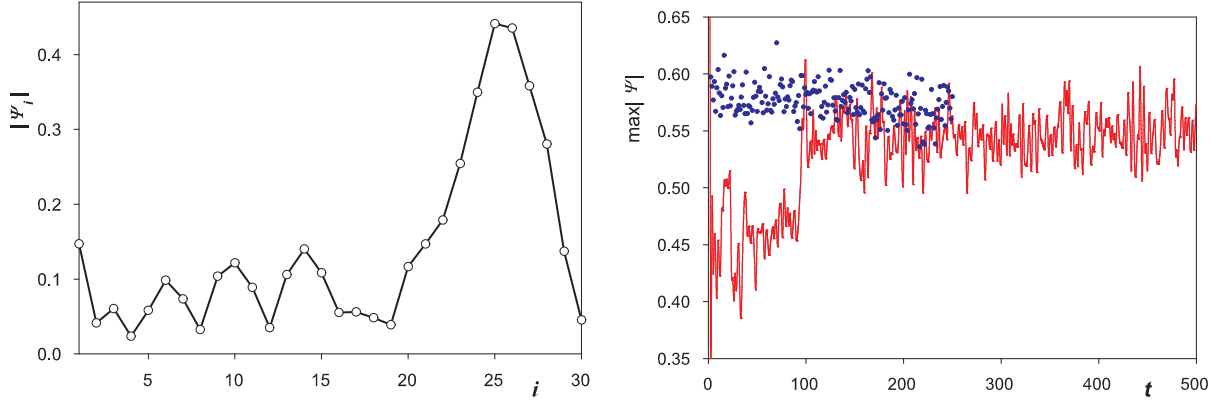


FIG. 6: a) Snapshot of the polaron wave function at time $t = 134$. $\alpha^2 = 2, N = 30, \tilde{e}_{25} = 1.5, \tilde{\alpha}_{25} = 0.1$. b) Maximal value of the wave function (in absolute value) *vs.* time. Solid line for $\tilde{\alpha} = 0.1$, dots for $\tilde{\alpha} = 1$. Every point is the result of averaging on the time interval $t = 1.25$. $N = 30, \alpha^2 = 2$.

and after induction period $t \approx 100$ for $\tilde{\alpha} = 0.1$.

There exists one more interesting case of the wave function evolution at some special choice of parameters. If parameter $\tilde{e} = 0$ (absence of the diagonal disorder) and only one hopping integral differs from the others, then it is the case when the lattice does not influence the electron evolution (as discussed above). The usual “hopping” dynamics on the homogeneous lattice will be observed. Let only first site differs from the others by the hopping constant $\tilde{t}_1 \neq t$ (see (2)) and the wave function is localized on the site $i = 1$ at the initial time $t = 0$. Naturally, no polaron is formed as the lattice does not influence the electron dynamics. But there exists the phenomenon of the periodic returning of the wave function to the first site. This phenomenon is related with the final lattice size and is shown in Fig. 7. Time is measured in “electronic” time units $\tilde{h}t$ which are related to dynamical time units by the dimensionless Planck’s constant $\tilde{h} = 0.0125$ (see above).

This problem (in very simple formulation) reminds experiments on the photoinduced charge transfer from intercalated metal complex to the DNA chain [42], and the value \tilde{t}_1 reflects the interaction of the ligand with the DNA bases.

Some interesting effects are experimentally observed: “chemistry at a distance” [43] and “ping-pong electron transfer” [44]. Our results can help to elucidate some experimental results which has no satisfactory interpretation yet [2]. Particularly the detailed analysis of

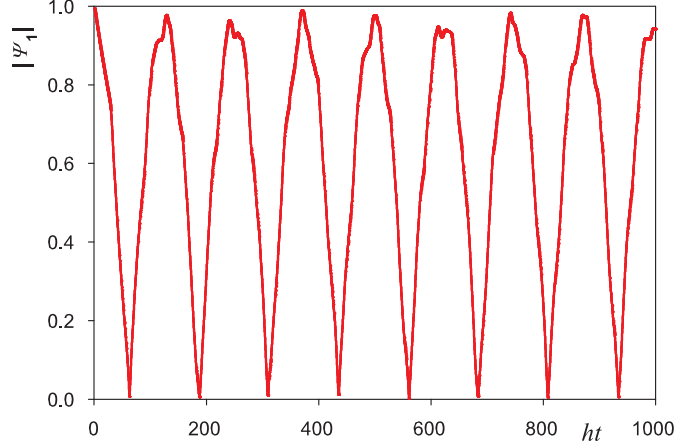


FIG. 7: Absolute value of the amplitude of the wave function on the first site. $N = 30, \tilde{t}_1 = 0.1$.

the “electronic ping-pong” will be given in our next paper where moving polarons will be considered.

The polaron behavior and wave function evolution were considered at zero temperature till now. The kinetic energy of thermal fluctuation can be rather high at ambient temperatures, and the polaronic time of life can be limited due to interactions with these fluctuations. Below we consider the evolution of the wave function at finite temperatures.

The following problem was solved numerically to find out the role of temperature. The stationary polaron was formed at the lattice center, as described in the previous section. Then the lattice was thermalized from its ends (Langevine random forces with friction) to achieve the necessary temperature. If the temperature is high enough, the polaron is destroyed rather soon. We monitor the maximal value of the squared absolute value of the wave function amplitude on the lattice, computing its averaged value over time interval $t = 50$. In the beginning this value is close to ~ 0.4 , what approximately corresponds to the squared maximum of amplitude for the standing polaron. Then this maximum falls down to ~ 0.1 at some time τ . This time corresponds to the polaron life time. When temperature decreases, τ increases. Life time τ *vs.* temperature is shown in Fig. 8

Of course, there no any firm basis to make a conclusion that the found temperature T_0 is the true critical temperature. Sooner this temperature should be determined by the lattice length N and the parameter α of electron-phonon interaction. It seems reasonable that the “critical” temperature should decrease with the growth of the lattice length N and

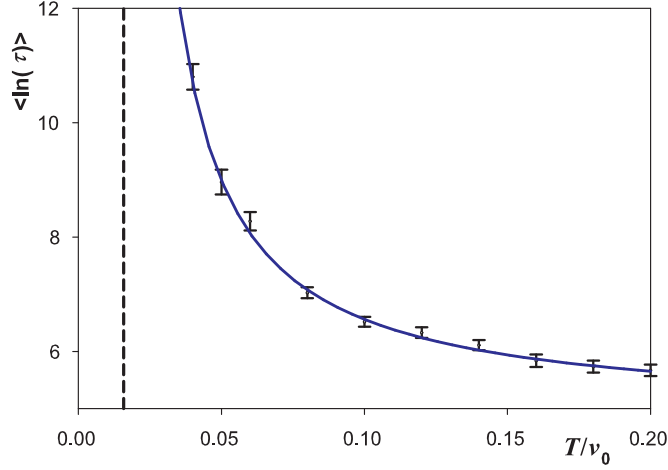


FIG. 8: Polaron time of life τ vs. the temperature. Temperature is measured in units of energy ($v_0 = 0.3$ eV for DNA). Solid line is the hyperbolic fitting $\lg(\tau) = a + b/(T - T_0)$, where a, b are some parameters, and T_0 is the “critical” temperature. Dashed line shows the asymptotic value $T_0 \approx 0.016$. Error bars correspond averaging over 20 random trajectories.

decreasing parameter α .

VI. CONCLUSIONS

Analytical expressions for the large- and small-radius polarons are derived in the present paper. The polaron radius is determined by the parameter α of the electron-phonon interaction in the SSH model: polaron is small at $\alpha \gtrsim 0.6$. The solution for the wave function of small-radius polaron represents a series where the first three terms are the solution of the system of algebraic equations and the next terms are geometrical progression. This form of solution is explained by the exponential decay of the wave function with increasing distance from the polaron center: $\psi_{i+1}/\psi_i = g = \text{const}$. For the large-radius polaron an analytical expression is derived in the continuous approximation. This solution reminds the solutions of some nonlinear equations (nonlinear Schrödinger, modified Korteweg – de Vries). Good agreement between analytical solutions and numerical simulation is obtained.

The considered simple model can help to explain existing experiments on the long range

coherent charge transfer in DNA.

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